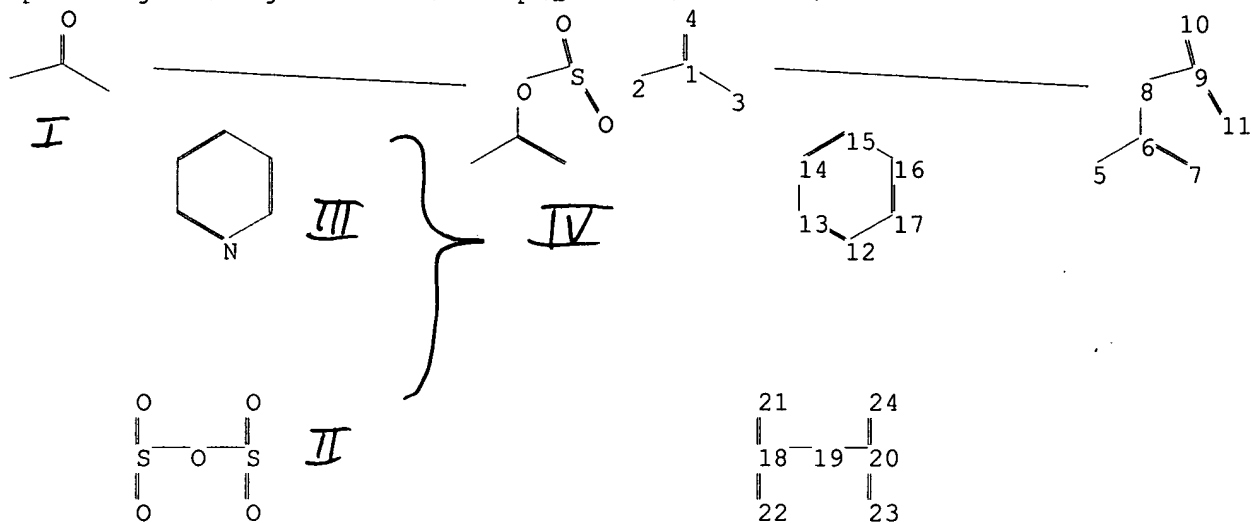


identification.

=&gt;

Uploading C:\Program Files\Stnexp\Queries\10518492\1.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 18 19 20 21 22 23 24

ring nodes :

12 13 14 15 16 17

chain bonds :

1-2 1-3 1-4 5-6 6-7 6-8 8-9 9-10 9-11 18-19 18-21 18-22 19-20 20-23 20-24

ring bonds :

12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

1-4 6-8 8-9 9-10 9-11 18-19 18-21 18-22 19-20 20-23 20-24

exact bonds :

1-2 1-3 5-6 6-7

normalized bonds :

12-13 12-17 13-14 14-15 15-16 16-17

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS

19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

fragments assigned product role:

containing 5

fragments assigned reactant/reagent role:

containing 1

containing 12

containing 18  
node mappings:  
1:6 4:8 2:5 3:7

L1 STRUCTURE UPLOADED

=> d  
L1 HAS NO ANSWERS  
L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> d  
L1 HAS NO ANSWERS  
L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full  
FULL SEARCH INITIATED 13:03:26 FILE 'CASREACT'  
SCREENING COMPLETE - 278 REACTIONS TO VERIFY FROM

52 DOCUMENTS

100.0% DONE 278 VERIFIED 22 HIT RXNS  
SEARCH TIME: 00.00.01

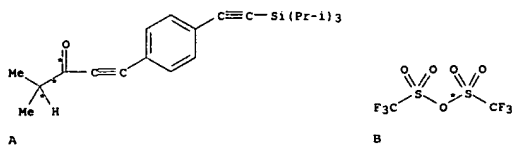
9 DOCS

L2 9 SEA SSS FUL L1 ( 22 REACTIONS)

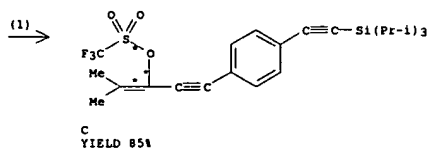
=> d ibib abs hit 1-9

L2 ANSWER 1 OF 9 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 143:7446 CASREACT  
 TITLE: Synthesis and characterization of cross-conjugated oligo(phenylene enynylene)s  
 AUTHOR(S): Cho, Joon; Zhao, Yuming; Tykwinski, Rik R.  
 CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.  
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (4), 142-150  
 CODEN: AGFUAR  
 URL: [http://www.arkat-usa.org/ark/journal/2005/I04\\_2efirov/1369/1369.pdf](http://www.arkat-usa.org/ark/journal/2005/I04_2efirov/1369/1369.pdf)  
 PUBLISHER: Arkat USA Inc.  
 DOCUMENT TYPE: Journal; (online computer file)  
 LANGUAGE: English  
 AB The synthesis and characterization of a series of cross-conjugated oligo(phenylene enynylene)s via the Sonogashira protocol is reported.  
 The structural properties of these oligomers have been established by <sup>1</sup>H and <sup>13</sup>C NMR and IR spectroscopies, as well as mass spectrometry. Their electronic absorption and emission behavior has been investigated via UV/Vis and fluorescence spectroscopy. The results of this study demonstrate that electronic communication along the conjugated framework of these oligomers is limited due to the presence of a cross-conjugated enyne framework and arylene fragments.  
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(1) OF 28 ...A + B ==> C...

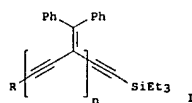


L2 ANSWER 1 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1) RCT A 052459-04-0, B 358-23-6  
 RGT D 38222-03-2 Me-(t-Bu)2-pyridine  
 PRO C 052459-03-7  
 SOL 75-09-2 CH2Cl2  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 0 deg C -> room temperature  
 SUBSTAGE(3) 4 hours, room temperature  
 NTE Sonogashira coupling

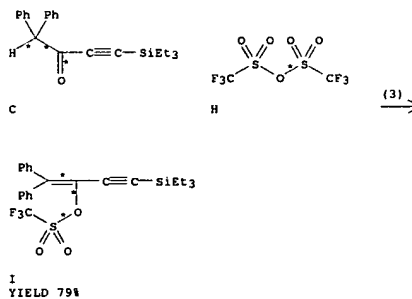
L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 142:279793 CASREACT  
 TITLE: Synthesis, structure, and nonlinear optical properties of cross-conjugated perphenylated iso-polydiacetylenes  
 AUTHOR(S): Zhao, Yuming; Slepkov, Aaron D.; Akoto, Clement Osei; McDonald, Robert; Hegmann, Frank A.; Tykwinski, Rik  
 R. Department of Chemistry, Memorial University of Newfoundland, St. John's, NL, A1B 3X7, Can.  
 CORPORATE SOURCE: Chemistry--A European Journal (2005), Volume Date 2004, 11(1), 321-329  
 SOURCE: CODEN: CEUJED; ISSN: 0947-6539  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Monodisperse, cross-conjugated perphenylated iso-polydiacetylene (iso-PDA) oligomers I (R = Me3Si, n = 1; R = Et3Si; n = 2, 3, 5, 7, 9, 11, 13, 15) have been synthesized by using a palladium-catalyzed cross-coupling protocol. Structural characteristics elucidated by x-ray crystallog. anal. demonstrate a non-planar backbone conformation for the oligomers due to the steric interactions between alkylidene Ph groups. The electronic absorption spectra of the oligomers show a slight red-shift of the maximum absorption wavelength as the chain length increases from dimer I (n = 2) to pentadecamer I (n = 15) a trend that has saturated by the stage of nonamer I (n = 9). Fluorescence spectroscopy confirms that the pendent Ph groups present on the oligomer framework enhance emission, and the relative emission intensity consistently increases as a function of chain length n. The mol. third-order nonlinearities,  $\chi^{(3)}$ , for this oligomer series have been measured via differential optical Kerr effect (DOKE) detection and show a superlinear increase as a function of the oligomer chain length n. Mol. modeling and spectroscopic studies suggest that iso-PDA oligomers I (n > 7) adopt a coiled, helical conformation in solution  
 REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

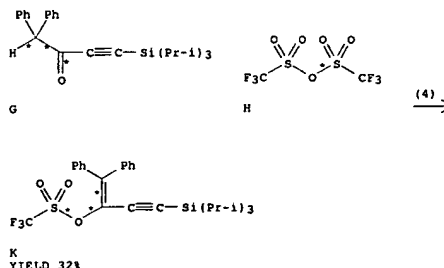
L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(3) OF 125 ...C + H ==> I...



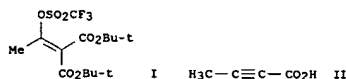
RX(3) RCT C 045725-73-7, H 358-23-6  
 RGT J 505-48-0 2,6-Di-t-Bu-pyridine  
 PRO I 339577-77-4  
 SOL 75-09-2 CH2Cl2  
 CON room temperature

RX(4) OF 125 ...G + H ==> K...



L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(4) RCT G 845725-74-9, H 358-23-6  
 RGT J 585-48-8 2,6-Di-t-Bu-pyridine  
 PRO K 845725-75-9  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON room temperature

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 141:140115 CASREACT  
 TITLE: Decarboxylative elimination of enol triflates as a general synthesis of acetylenes  
 AUTHOR(S): Fleming, Ian; Ramarao, Chandrashekar  
 CORPORATE SOURCE: Department of Chemistry, Cambridge, CB2 1EW, UK  
 SOURCE: Organic & Biomolecular Chemistry (2004), 2(10), 1504-1510  
 CODEN: OBCRAK; ISSN: 1477-0520  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

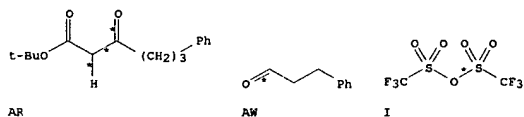


AB The enol trifluoromethanesulfonates of tert-Bu β-keto diesters and β-keto esters can be hydrolyzed to the corresponding carboxylic acids by dissoln. in trifluoroacetic acid. The dicarboxylic acids undergo mild decarboxylative elimination to give acetylenic acids in aqueous sodium bicarbonate solution at room temperature. Similarly, monocarboxylic acids give terminal and mid-chain acetylenes by refluxing in acetone with potassium carbonate. One of the substituents on the acetylenes can be Me, primary alkyl, secondary alkyl or ethynyl, and the other can be a carboxylic acid, hydrogen or primary alkyl, but the enol trifluoromethanesulfonates could not be prepared when one of the substituents was tert-Bu, nor when both substituents on the precursor to the acetylene were secondary alkyl. For example, reaction of trifluoromethanesulfonic acid anhydride with (acetyl)propanedioic acid bis(1,1-dimethylethyl) ester gave a desired enol triflate, [1-[(trifluoromethyl)sulfonyloxy]ethylidene]propanedioic acid bis(1,1-dimethylethyl) ester (I). Saponification of I gave the diacid, [1-[(trifluoromethyl)sulfonyloxy]ethylidene]propanedioic acid. Decarboxylation of the acid gave 2-butyneic acid (II).

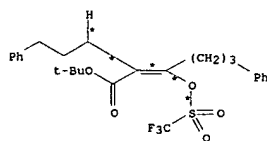
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(96) OF 118 COMPOSED OF RX(22), RX(26), RX(29)  
 RX(96) AR + AW + I ==> BK

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



3  
 STEPS  
 →



BK  
 YIELD 86%

RX(22) RCT AR 235087-24-8, AW 104-53-0

STAGE(1)  
 RGT AY 7550-45-0 TiCl<sub>4</sub>, AZ 110-86-1 Pyridine  
 SOL 109-99-9 THF, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 30 minutes, 0 deg C  
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)  
 RGT F 12125-02-9 NH<sub>4</sub>Cl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO AX 725340-58-9  
 NTE stereoselective, isomer mix.

RX(26) RCT AX 725340-58-9  
 RGT BF 1333-74-0 H<sub>2</sub>  
 PRO BE 235087-25-9  
 CAT 7440-05-3 Pd  
 SOL 67-56-1 MeOH  
 CON 24 hours, room temperature

RX(29) RCT BE 235087-25-9

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

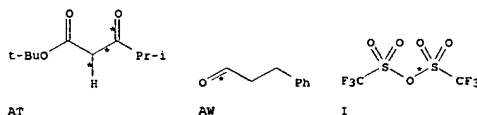
STAGE(1)  
 RGT L 7646-69-7 NaH  
 SOL 60-29-7 Et<sub>2</sub>O  
 CON 1 hour, 0 deg C

STAGE(2)  
 RCT I 358-23-6  
 CON SUBSTAGE(1) 1 hour, 0 deg C  
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)  
 RGT F 12125-02-9 NH<sub>4</sub>Cl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO BK 235087-28-2

RX(98) OF 118 COMPOSED OF RX(23), RX(27), RX(30)  
 RX(98) AT + AW + I ==> BL



AT

AW

I

3  
 STEPS  
 →

BL  
 YIELD 92%

RX(23) RCT AT 94250-54-1, AW 104-53-0

STAGE(1)  
 RGT AY 7550-45-0 TiCl<sub>4</sub>, AZ 110-86-1 Pyridine  
 SOL 109-99-9 THF, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 30 minutes, 0 deg C  
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)  
 RGT F 12125-02-9 NH<sub>4</sub>Cl  
 SOL 7732-18-5 Water  
 CON room temperature

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 PRO BA 725340-63-6  
 NTE stereoselective, isomer mix.

RX(27) RCT BA 725340-63-6  
 RGT BF 1333-74-0 H2  
 PRO BI 235087-26-0  
 CAT 7440-05-3 Pd  
 SOL 67-56-1 MeOH  
 CON 24 hours, room temperature

RX(30) RCT BI 235087-26-0

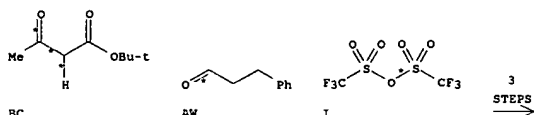
STAGE(1)  
 RGT L 7646-69-7 NaH  
 SOL 60-29-7 Et2O  
 CON 1 hour, 0 deg C

STAGE(2)  
 RCT I 358-23-6  
 CON SUBSTAGE(1) 1 hour, 0 deg C  
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)  
 RGT F 12125-02-9 NH4Cl  
 SOL 7732-18-5 Water  
 CON room temperature

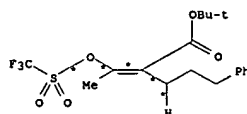
PRO BL 235087-30-6

RX(100) OF 118 COMPOSED OF RX(25), RX(28), RX(31)  
 RX(100) BC + AW + I ==> BM



L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 PRO BM 725340-88-5

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BM  
 YIELD 71%

RX(25) RCT BC 1694-31-1, AW 104-53-0

STAGE(1)  
 RGT AY 7550-45-0 TiCl4, AZ 110-86-1 Pyridine  
 SOL 109-99-9 THF, 75-09-2 CH2Cl2  
 CON SUBSTAGE(1) 30 minutes, 0 deg C  
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)  
 RGT F 12125-02-9 NH4Cl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO BD 725340-53-4  
 NTE stereoselective, isomer mix.

RX(28) RCT BD 725340-53-4  
 RGT BF 1333-74-0 H2  
 PRO BJ 725340-75-0  
 CAT 7440-05-3 Pd  
 SOL 67-56-1 MeOH  
 CON 24 hours, room temperature

RX(31) RCT BJ 725340-75-0

STAGE(1)  
 RGT L 7646-69-7 NaH  
 SOL 60-29-7 Et2O  
 CON 1 hour, 0 deg C

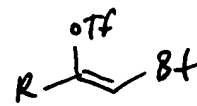
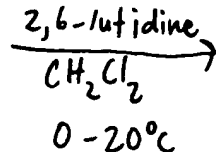
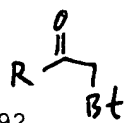
STAGE(2)  
 RCT I 358-23-6  
 CON SUBSTAGE(1) 1 hour, 0 deg C  
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)  
 RGT F 12125-02-9 NH4Cl  
 SOL 7732-18-5 Water  
 CON room temperature

L2 ANSWER 4 OF 9 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 140:111001 CASREACT  
 TITLE: Fragmentations of (E)- and (Z)-isomers of 2-methylbuten-1-yl(aryl) iodonium triflates:  
 competing mechanisms for enol triflate formation  
 AUTHOR(S): Hinkle, Robert J.; Mikowski, Ann M.  
 CORPORATE SOURCE: Dep. Chem., The College of William and Mary, Williamsburg, VA, 23187-8795, USA  
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (6), 201-212  
 CODEN: AGFUAR  
 URL: <http://www.arkat-usa.org/ark/journal/2003/Varvogli15/AV-745A/745A.pdf>  
 PUBLISHER: Arkat USA Inc.  
 DOCUMENT TYPE: Journal; (online computer file)  
 LANGUAGE: English  
 AB We examined fragmentation reactions of (E)- and (Z)-2-methylbuten-1-yl(aryl)iodonium triflates (aryl = C6H5-, 4-(CF3)C6H4-, 3,5-(CF3)2C6H4-) to afford aryl iodides and six enol triflates. Four of these vinyl triflates involve alkyl migrations followed by triflate trapping of secondary vinyl cations whereas two do not involve migrations. Fragmentation rates in dry, neutral CDCl3 were determined as were the distributions of enol triflate products. The ratios of rate consts. for the (E)-/(Z)- isomers ranged between 5.0 and 8.5 and, in all salts, the rearranged enol triflate derived from migration of the alkyl moiety trans- to the aryl-iodonio- nucleofuge was observed in the greatest quantities. These data indicate that the fragmentation rates are significantly determined by the migratory aptitude of the trans-β-alkyl substituent and departure of the aryl-iodonio-nucleofuge occurs by anchimeric assistance. The ratios of inverted "unrearranged" enol triflate products were greater for the (Z)-isomers of the iodonium salt precursors indicating that steric effects play a role and implies that these inverted, unrearranged products are derived from in plane (σ\*) SN2 reaction. The presence of the remaining, retained, unrearranged enol triflate can be explained by a ligand coupling mechanism (π\* SN2) and the fragmentation mechanism(s) do not require the intermediacy of a primary vinyl cation.  
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(5) OF 10 2 H + 2 O ==> P + Q

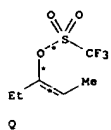
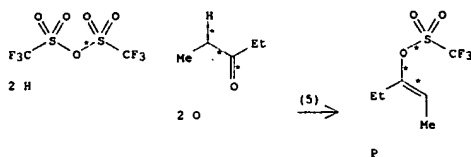
10/518,492



05/05/2006

L2 ANSWER 4 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(5) RCT H 358-23-6, O 96-22-0

STAGE(1)

RGT L 585-46-8 2,6-Di-t-Bu-pyridine

SOL 75-09-2 CH2Cl2

CON 12 hours, room temperature

STAGE(2)

SOL 109-66-0 Pentane

PRO P 52149-31-2, Q 52149-30-1

NTE stereoselective

experiment  
P. 5608

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 133:257018 CASREACT

TITLE: One-Carbon Homologation of Carboxylic Acids via BtCH2TMS: A Safe Alternative to the Arndt-Eistert Reaction

AUTHOR(S): Katritzky, Alan R.; Zhang, Suoming; Mostafa Hussein, Abdel Haleem; Fang, Yunfeng; Steel, Peter J.

CORPORATE SOURCE: Center for Heterocyclic Compounds Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA

SOURCE: 5606-5612

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Carboxylic acids are converted into the corresponding homologated acids or

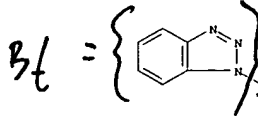
esters, using easily available 1-(trimethylsilylmethyl)benzotriazole as a one-carbon synthon. The effectiveness of the reaction has been investigated on six aryl and seven alkyl carboxylic acids.

REFERENCE COUNT: 39 THERE ARE 39 CITATIONS AVAILABLE FOR THIS

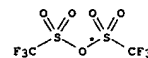
FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(20) OF 153 ...P + AC ==&gt; AL...

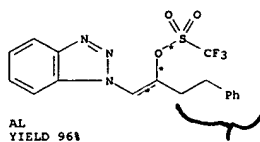
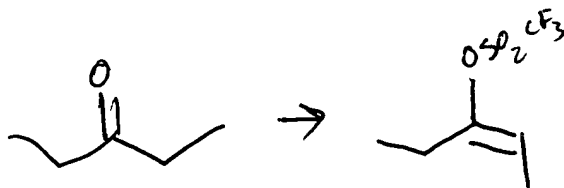


P



(20)

Table 1,  
page 5607



RX(20) RCT P 361379-11-5, AC 358-23-6

RGT AE 108-48-5 2,6-Lutidine

ex (g) Table 1



L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

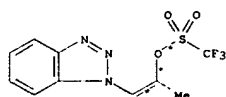
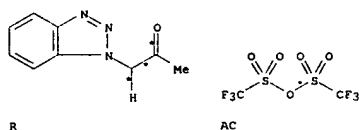
(Continued)

PRO AL 361379-20-6

SOL 75-09-2 CH2Cl2

NTE stereoselective

RX(21) OF 153 ...R + AC ==&gt; AN...



RX(21) RCT R 64882-50-4, AC 358-23-6

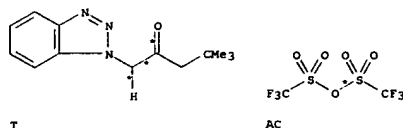
RGT AE 108-48-5 2,6-Lutidine

PRO AM 361379-21-7

SOL 75-09-2 CH2Cl2

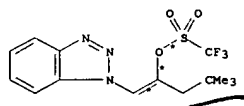
NTE stereoselective

RX(22) OF 153 ...T + AC ==&gt; AN...



L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(22) RCT T 314765-22-5, AC 358-23-6

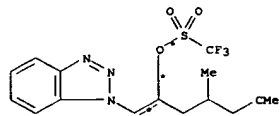
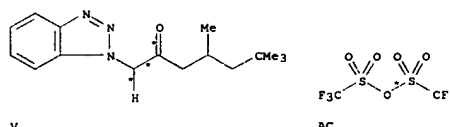
RGT AE 108-48-5 2,6-Lutidine

PRO AN 361379-22-8

SOL 75-09-2 CH2Cl2

NTE stereoselective

RX(23) OF 153 ...V + AC ==&gt; AO...



RX(23) RCT V 361379-13-7, AC 358-23-6

RGT AE 108-48-5 2,6-Lutidine

PRO AO 361379-23-9

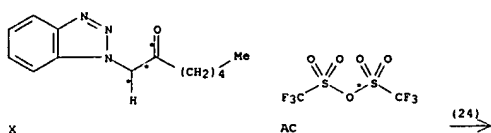
SOL 75-09-2 CH2Cl2

NTE stereoselective

RX(24) OF 153 ...X + AC ==&gt; AP...

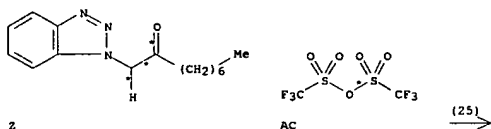
ex (j)

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AP  
YIELD 94%

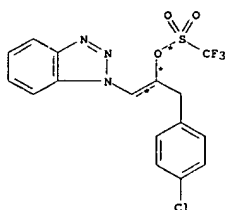
RX(24) RCT X 189343-44-0, AC 358-23-6  
 RGT AE 108-48-5 2,6-Lutidine  
 PRO AP 361379-24-0  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 NTE stereoselective

RX(25) OF 153 ...E + AC ==&gt; AQ...



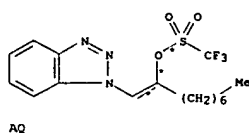
Z

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AR  
YIELD 82%

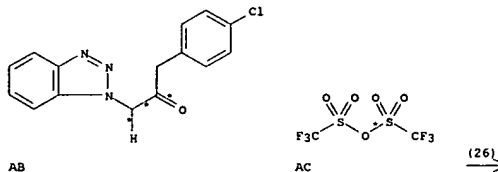
RX(26) RCT AB 306990-72-7, AC 358-23-6  
 RGT AE 108-48-5 2,6-Lutidine  
 PRO AR 361379-26-2  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 NTE stereoselective

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AQ  
YIELD 90%

RX(25) RCT Z 304459-92-5, AC 358-23-6  
 RGT AE 108-48-5 2,6-Lutidine  
 PRO AQ 361379-25-1  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 NTE stereoselective

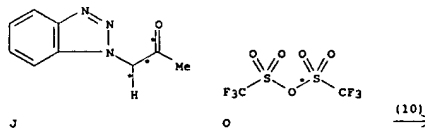
RX(26) OF 153 ...AB + AC ==&gt; AR



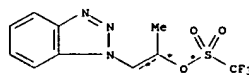
AB

L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 134:71356 CASREACT  
 TITLE: BtCH<sub>2</sub>TMS-Assisted Homologation of Carboxylic Acids: A Safe Alternative to the Arndt-Eistert Reaction  
 AUTHOR(S): Katritzky, Alan R.; Zhang, Suoming; Fang, Yunfeng  
 CORPORATE SOURCE: Center for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA  
 SOURCE: Organic Letters (2000), 2(24), 3789-3791  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB One-carbon homologation of carboxylic acids is achieved by (i) treatment of an acyl chloride with 1-[(trimethylsilyl)methyl]-1H-1,2,3-benzotriazole (BtCH<sub>2</sub>TMS) to afford N-(acylmethyl)benzotriazoles, followed by (ii) conversion with triflic anhydride into RC(OTf):CHBt, and (iii) the subsequent reaction with NaOCH<sub>3</sub> followed by 1N HCl to afford esters RCH<sub>2</sub>CO<sub>2</sub>R' in overall yields of 50-70%. For the aliphatic compds., treatment with p-toluenesulfonic acid followed by TBAF/THF afforded acids RCH<sub>2</sub>COOH.  
 REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS  
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(10) OF 69 ...J + O ==&gt; V...



J

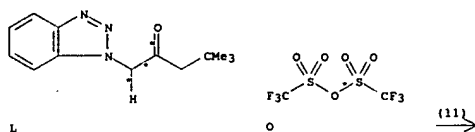
V  
YIELD 88%

RX(10) RCT J 64882-50-4, O 358-23-6  
 STAGE(1)  
 RGT Q 108-48-5 2,6-Lutidine  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

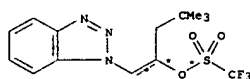
L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
STAGE(2)  
SOL 110-54-3 Hexane

PRO V 314765-31-6

RX(11) OF 69 ...L + O ==> W...



L



W  
YIELD 95%

RX(11) RCT L 314765-22-5, O 358-23-6

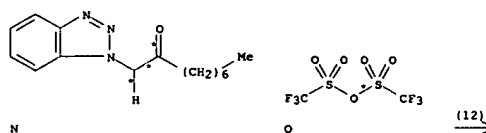
STAGE(1)  
RGT Q 108-48-5 2,6-Lutidine  
SOL 75-09-2 CH2Cl2

STAGE(2)  
SOL 110-54-3 Hexane

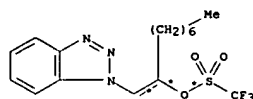
PRO W 314765-33-8

RX(12) OF 69 ...N + O ==> X...

L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



N



X  
YIELD 90%

RX(12) RCT N 304459-92-5, O 358-23-6

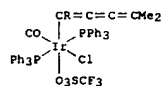
STAGE(1)  
RGT Q 108-48-5 2,6-Lutidine  
SOL 75-09-2 CH2Cl2

STAGE(2)  
SOL 110-54-3 Hexane

PRO X 314765-35-0

L2 ANSWER 7 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

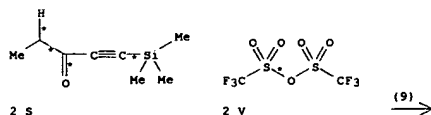
ACCESSION NUMBER: 106:138608 CASREACT  
TITLE: Kinetics, stereochemistry, and mechanism of interaction of Vaska's complex with ethynylvinyl triflates. Formation of novel  $\sigma$ -butatrienyliridium compounds  
AUTHOR(S): Stang, Peter J.; Dixit, Vandana; Schiavelli, Melvyn D.; Drees, Paul  
CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, 84112, USA  
SOURCE: Journal of the American Chemical Society (1987), 109(4), 1150-6  
CODEN: JACSAT; ISSN: 0002-7863  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

AB The reaction of Vaska's complex  $[(\text{Ph}_3\text{P})_2\text{Ir}(\text{CO})(\text{Cl})]$  with  $\text{Me}_2\text{C}=\text{C}(\text{O}_2\text{SCF}_3)\text{C}\equiv\text{C}\text{R}$  ( $\text{R} = \text{H}, \text{D}, \text{Me}, \text{Ph}, \text{SiMe}_3$ ) was investigated. Oxidative addition readily occurs in benzene or toluene at room temperature to give hexacoordinate Ir(III) butatrienyl complexes I ( $\text{R} = \text{same}$ ). Rate studies indicate steric inhibition by bulky substituents on the terminal acetylenic C and give high neg. entropies of activation. The reaction occurs with complete (or nearly complete) retention of olefin stereochem. A two-step  $\text{S}_\text{N}2$  process with syn approach of the incoming Ir nucleophile is proposed to account for these observations.

RX(9) OF 28 ...2 S + 2 V ==> M + P...

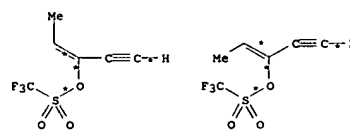


2 S

2 V

(9)

L2 ANSWER 7 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



M  
YIELD 77% (45)

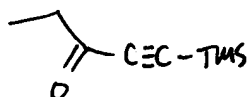
P  
YIELD 77% (75)

RX(9) RCT S 10307-50-1, V 358-23-6  
RGT W 30222-03-2 Me-(t-Bu)2-pyridine  
PRO M 106211-71-6, P 106211-72-7  
SOL 75-09-2 CH2Cl2



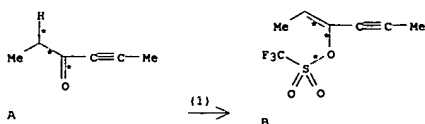
references Synthesis, 1979, 438  
(Stang et al.)

Synthesis, 1982, 85 (105)



L2 ANSWER 8 OF 9 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 104:148249 CASREACT  
 TITLE: The preparation of unsymmetrical diacetylenes from alkenynyl triflates  
 AUTHOR(S): Stang, Peter J.; Dixit, Vandana  
 CORPORATE SOURCE: Chem. Dep., Univ. Utah, Salt Lake City, UT, 84112, USA  
 SOURCE: Synthesis (1985), (10), 962-3  
 CODEN: SYNTBF; ISSN: 0039-7881  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB RC.tplbond.CC(O3SCF3):CHMe (I; R = Me, Ph) were converted in 85% yield to RC.tplbond.CC.tplbond.CMe by treatment with 2,6-(Me3C)2C6H3OK in glyme. Me3SiC.tplbond.CC.tplbond.CMe was similarly prepared in 45% yield by treating I (R = Me3Si) with (Me2CH)2NLi in glyme. I were prepared by treating RC.tplbond.CCOCH2Me with (CF3SO2)2O in the presence of 2,6-di-tert-butyl-4-methylpyridine.

RX(1) OF 9 A ==> B...



RX(1) RCT A 10575-41-4  
 RGT C 38222-83-2 Me-(t-Bu)2-pyridine, D 358-23-6  
 (F3CSO2)2O  
 PRO B 101160-51-4  
 SOL 75-09-2 CH2Cl2

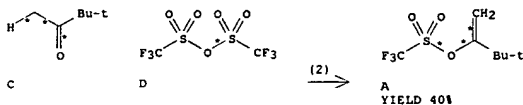
RX(2) OF 9 F ==> G...



RX(2) RCT F 19307-74-5  
 RGT C 38222-83-2 Me-(t-Bu)2-pyridine, D 358-23-6

L2 ANSWER 9 OF 9 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 80:82004 CASREACT  
 TITLE: Vinyl triflates in synthesis. I.  
 AUTHOR(S): Hargrove, Robert J.; Stang, Peter J.  
 CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, USA  
 SOURCE: Journal of Organic Chemistry (1974), 39(4), 581-2  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The elimination of CF3SO3H from Me3CC(O3SCF3):CH2 (I) to give MeCC.tplbond.CH is catalyzed by pyridine. Pinacolone reacts with (CF3SO2)2O to give I.

RX(2) OF 3 C + D ==> A...



RX(2) RCT C 75-97-8, D 358-23-6  
 RGT E 110-86-1 Pyridine  
 PRO A 27701-32-2  
 SOL 56-23-5 CCl4  
 NTE Classification: Isomerisation; O-Sulphonation; # Conditions: triflic anhydride; CCl4 pyridine; 15 deg 60h

soln of  
 (c)  
 0.02 mol  
 + pyridine  
 0.022 mol

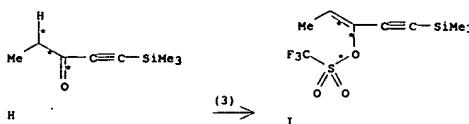


-22°C  
 15 min then warm to 15°C for 60 hr.

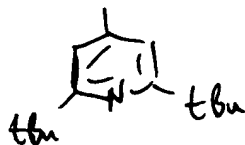
add in TF2O (0.022 mol)

L2 ANSWER 8 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 (F3CSO2)2O  
 PRO G 101160-52-5  
 SOL 75-09-2 CH2Cl2

RX(3) OF 9 H ==> I...



RX(3) RCT H 18387-58-1  
 RGT C 38222-83-2 Me-(t-Bu)2-pyridine, D 358-23-6  
 (F3CSO2)2O  
 PRO I 101160-53-6  
 SOL 75-09-2 CH2Cl2



methods in Stang et al.

Synthesis 1979, 438

references - Dueber et al. Angew. Chem  
 Int. Ed. Engl. 9, 521 (1970)

1D) { Stang & Dueber, Org. Syn.  
 54, 79 (1974)